

# Thermochemical Properties of Xanthine and Hypoxanthine Revisited

Emel'yanenko V., Zaitsau D., Verevkin S.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

---

## Abstract

© 2017 American Chemical Society. The standard molar enthalpies of formation of xanthine and hypoxanthine were measured by using high-precision combustion calorimetry. The standard molar enthalpies of sublimation of these compounds at 298.15 K were derived by the quartz-crystal microbalance technique. Limited thermodynamic data available in the literature are compared with our new experimental data. In addition, we use the G4 method to calculate the molar enthalpies of formation of xanthine and hypoxanthine in the gas phase. There is good agreement between the evaluated experimental data and the quantum-chemical calculations. (Chemical Equation Presented).

<http://dx.doi.org/10.1021/acs.jced.7b00085>

---

## References

- [1] Stiehler, R. D.; Huffman, H. M. Thermal Data. IV. The Heats of Combustion of Adenine, Hypoxanthine, Guanine, Xanthine, Uric Acid, Allantoin and Alloxan J. Am. Chem. Soc. 1935, 57 (9) 1734-1740 10.1021/ja01312a071
- [2] Stiehler, R. D.; Huffman, H. M. Thermal Data. V. The Heat Capacities, Entropies and Free Energies of Adenine, Hypoxanthine, Guanine, Xanthine, Uric Acid, Allantoin and Alloxan J. Am. Chem. Soc. 1935, 57 (9) 1741-1743 10.1021/ja01312a072
- [3] Teplitskii, A. B.; Yanson, I. K. Effect of Substituents on the Heat of Sublimation of Nucleic Acid Nitrogenous Bases Biofizika 1975, 20 (2) 189-193
- [4] Emel'yanenko, V. N.; Verevkin, S. P.; Notario, R. Thermochemistry of Uracil and Thymine Revisited J. Chem. Thermodyn. 2015, 87, 129-135 10.1016/j.jct.2015.03.015
- [5] Emel'yanenko, V. N.; Zaitsau, D. H.; Shoifet, E.; Meurer, F.; Verevkin, S. P.; Schick, C.; Held, C. Benchmark Thermochemistry for Biologically Relevant Adenine and Cytosine. A Combined Experimental and Theoretical Study J. Phys. Chem. A 2015, 119 (37) 9680-9691 10.1021/acs.jpca.5b04753
- [6] Beckhaus, H.-D.; Kratt, G.; Lay, K.; Geiselmann, J.; Rüchardt, C.; Kitschke, B.; Lindner, H. J. Thermolabile Kohlenwasserstoffe, XIII. 3,4-Dicyclohexyl-3,4-Dimethylhexan - Standardbildungsenthalpie, Thermische Stabilität Und Struktur Chem. Ber. 1980, 113 (11) 3441-3455 10.1002/cber.19801131104
- [7] Wieser, M. E.; Holden, N.; Coplen, T. B.; Böhlke, J. K.; Berglund, M.; Brand, W. A.; De Bièvre, P.; Gröning, M.; De Loss, R.; Meija, J. et al. Atomic Weights of the Elements 2011 (IUPAC Technical Report) Pure Appl. Chem. 2013, 85 (5) 1047-1078 10.1351/PAC-REP-13-03-02
- [8] Hubbard, W. N.; Scott, D. W.; Waddington, G.; Rossini, F. D. Standard States and Corrections for Combustions in a Bomb at Constant Vol. In Experimental thermochemistry: measurement of heats of reaction; Interscience Publishers: New York, 1956; Vol. 1, pp 75-128.
- [9] Verevkin, S. P.; Zaitsau, D. H.; Emel'yanenko, V. N.; Heintz, A. A New Method for the Determination of Vaporization Enthalpies of Ionic Liquids at Low Temperatures J. Phys. Chem. B 2011, 115 (44) 12889-12895 10.1021/jp207397v
- [10] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; et al., Gaussian 09, revision D.01. Gaussian, Inc.: Wallingford, CT, USA, 2016.

- [11] Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-4 Theory J. Chem. Phys. 2007, 126 (8) 84108-84112 10.1063/1.2436888
- [12] Verevkin, S. P.; Emel'yanenko, V. N.; Notario, R.; Roux, M. V.; Chickos, J. S.; Liebman, J. F. Rediscovering the Wheel. Thermochemical Analysis of Energetics of the Aromatic Diazines J. Phys. Chem. Lett. 2012, 3 (23) 3454-3459 10.1021/jz301524c
- [13] McQuarrie, D. A. Statistical Mechanics; Harper & Row: New York, 1975.
- [14] Cox, J. D.; Wagman, D. D.; Medvedev, V. A. CODATA Key Values for Thermodynamics; Hemisphere Pub. Corp.: New York, 1989.
- [15] Olofsson, G. Assignment of Uncertainties. In Combustion Calorimetry; Pergamon, 1979; Chapter 6, pp 137-161.
- [16] Chickos, J. S.; Acree, W. E., Jr. Enthalpies of Sublimation of Organic and Organometallic Compounds. 1910-2001 J. Phys. Chem. Ref. Data 2002, 31 (2) 537-698 10.1063/1.1475333
- [17] Verevkin, S. P.; Emel'yanenko, V. N.; Varfolomeev, M. A.; Solomonov, B. N.; Zherikova, K. V.; Melkhanova, S. V. Thermochemistry of Dihalogen-Substituted Benzenes: Data Evaluation Using Experimental and Quantum Chemical Methods J. Phys. Chem. B 2014, 118 (49) 14479-14492 10.1021/jp5097844
- [18] Wangler, A.; Canales, R.; Held, C.; Luong, T. Q.; Winter, R.; Zaitsau, D. H.; Verevkin, S. P.; Sadowski, G. Towards a Quantitative Understanding of Co-Solvent Effects on Rate and Equilibrium Data of Enzymatic Reactions. Angew. Chem. 2017, submitted
- [19] Marsh, K. N.; Månsson, M. Standard Molar Enthalpies of Formation of Triethoxymethane and Tetraethoxymethane by Rotating Bomb Calorimetry J. Chem. Thermodyn. 1985, 17 (10) 995-1002 10.1016/0021-9614(85)90014-X
- [20] Duarte-Garza, H. A.; Stouffer, C. E.; Hall, K. R.; Holste, J. C.; Marsh, K. N.; Gammon, B. E. Experimental Critical Constants, Vapor Pressures, and Vapor and Liquid Densities for Pentafluoroethane (R-125) J. Chem. Eng. Data 1997, 42 (4) 745-753 10.1021/je960362f
- [21] Curtiss, L. A.; Redfern, P. C.; Raghavachari, K. Gaussian-4 theory J. Chem. Phys. 2007, 126, 084108 10.1063/1.2436888